

Optical properties of ternary alloys MgZnO in infrared spectrum

E.F. Venger¹, I.V. Venger¹, N.O. Korsunskaya¹, L.Yu. Melnichuk², O.V. Melnichuk², L.Yu. Khomenkova¹

¹ V. Lashkaryov Institute of Semiconductor Physics, NAS of Ukraine, 41, prosp. Nauky, 03680 Kyiv, Ukraine

² Mykola Gogol State University of Nizhyn, 2, Hrafka str., 16600 Nizhyn, Ukraine

E-mail: mov310310@gmail.com

Abstract. Properties of thin films of ternary alloys $Mg_xZn_{1-x}O$ on the optically-anisotropic Al_2O_3 substrates in the area of “residual rays” of film and substrate are first investigated using the method of infrared spectroscopy and dispersion analysis of reflection coefficients. It was established that the changes in thickness of film and content of Mg substantially deform the spectrum of reflection in the area of “residual rays” of film and substrate, decrease the reflectivity. First by means of Kramers–Kronig relations with use of the method of dispersion analysis of infrared reflection spectra, the static dielectric constant of $Mg_xZn_{1-x}O$ structure has been obtained at different values of x , when orientation is $E \perp C$. It was ascertained that the $Mg_xZn_{1-x}O/Al_2O_3$ structures are well modelled when using the mutually agreed parameters, obtained earlier for the single crystals of magnesium oxide, zinc oxide and leucosapphire at the orientation $E \perp C$. It was theoretically shown and experimentally grounded the assurance of the obtained optical parameters of $Mg_xZn_{1-x}O$ films by the non-destructive method of infrared spectroscopy in the wide spectral range. The obtained results are well agreed with the literature data.

Keywords: optical properties, ternary alloys, MgZnO, infrared spectrum, infrared spectroscopy, dispersion analysis of reflection coefficients.

doi: <https://doi.org/10.15407/spqeo21.04.417>

PACS 78.20.Ci, 78.40.-q

Manuscript received 23.10.18; revised version received 15.11.18; accepted for publication 29.11.18; published online 03.12.18.

1. Introduction

Today zinc oxide (ZnO), due to its high radiation, chemical and thermal stability, is an enough applicable semiconductor in acousto-, opto- and nanoelectronics [1-4]. Zinc oxide is especially actual when making the transparent film electrodes for solar cells [5], and high binding energy of excitons (60 meV) in ZnO promotes laser generation at room temperature [1, 2]. A bandgap ($E_g = 3.37$ eV) allows to use ZnO for creation of detectors and filters in the ultraviolet range. In addition, zinc oxide found wide application for manufacturing gas sensors, light-emitting diodes, varistors, photocatalyzators for cleaning water and air *etc.* [5]. In its turn, ZnO films on Si and CdTe substrates have considerably subzero prime price and are perspective material for creation of antireflective, current-carrying layers in solar cells of large area [5-7].

Next to ZnO, there is another widely used material that has excellent characteristics in application, it is magnesium oxide (MgO). MgO is one of the most widespread natural minerals that is crystallized in the rocky structure of Earth at any pressures and temperatures [8]. The crystals of MgO are transparent,

fire and explosion undangerous, practically insoluble in water, however soluble in muriatic, sulphuric and vinegar acids. MgO has a high temperature of melting 2800 °C, that is why it is widely used as substrate material for the processes of growing thin films in modern microelectronic and optronic devices [8, 9].

In the works by Ye.F. Venger and coauthors [10-12], the analysis of both ZnO and MgO compounds was performed, which is a result of that ZnO is compound of semiconductor of family A^2B^6 , and MgO is usually examined as a widegap semiconductor close to dielectric, as its bandgap is 8.2 eV. MgO has a cubic structure like NaCl type. However, in spite of the fact that ZnO and MgO have different crystalline structures, zinc oxide has a hexagonal crystalline structure (wurtzite), and magnesium oxide – the cubic one, these two materials can be connected with each other, forming the $Mg_xZn_{1-x}O$ compound. The obtained ternary compound extends the limits of their application. First it was described in the works Kawasaki *et al.* [13], where the possibility to change optical and electrophysical properties of ternary alloys $Mg_xZn_{1-x}O$ by changing the bandgap in ZnO films was shown.

Thus, for the increase of E_g it needs to use the elements of the second group that are placed higher in the Mendeleev table, for example Mg [13], and for decrease – elements that are below, for example Cd [14]. In the dependence on the relative concentrations of Mg and Zn, ternary alloys $Mg_xZn_{1-x}O$ may have both hexagonal crystalline structure (wurtzite) and the cubic one. In the work [15], it was shown that at $x < 0.3$ hexagonal crystalline structure is inherent to $Mg_xZn_{1-x}O$ and bandgap changes from 3.4 up to 3.8 eV, which allows to use them for manufacturing substances for optoelectronics with the range of wavelengths from red up to deep ultraviolet. At $x > 0.3$, cubic crystalline structure is inherent to $Mg_xZn_{1-x}O$. Thus, due to the unique properties (high photo-response, high quantum yield of photo- and cathodoluminescence, presence of pyro- and piezoelectric effects *etc.*), $Mg_xZn_{1-x}O$ films belong to materials that provide a base for the various optoelectronic devices that were created with the use of volume and surface waves. Advantage of the devices based on $Mg_xZn_{1-x}O$ is their diminutiveness, high efficiency of operation in a wide frequency range, use in optics and optoelectronics, in light-emitting diodes for the ultraviolet spectral region, in laser diodes or sensors, as well as possibility of integration with other microelectronic elements [15-20].

However, data about study of undoped and strong doped films of $MgZnO$ at the concentrations of electrons from 10^{16} to $5 \cdot 10^{18} \text{ cm}^{-3}$ on the Al_2O_3 dielectric substrates by using the method of infrared spectroscopy of external reflection in the area of “residual rays” of film and substrate at the orientations $E \perp C$ and $E \parallel C$ in the literature is lighted up limit enough.

Attractiveness to research the ternary alloys $Mg_xZn_{1-x}O$ with the range of Mg^{2+} from 0 to 30% is keeping the hexagonal lattice and displaying the optically-anisotropic properties in the infrared spectrum. At $x > 30\%$, the cubic lattice of the considered ternary alloys is typical.

The aim of this work was to study optical properties of films of ternary alloys $Mg_xZn_{1-x}O$ on the optically-anisotropic Al_2O_3 substrates by means of the method of spectroscopy of external infrared reflection.

2. Samples and the method for measuring

Synthesis of the films was performed using the industrial modernized setup BY-1A and possibilities of computer controlling the technological parameters (temperature, pressure, position of shutters *etc.*). It was shown that the developed software allowed the operator to force setup into an operation mode, to synthesize automatically thin films (at the set temperature conditions, thickness, concentrations of free charge carriers *etc.*) and remove of setup from operation mode. The rate of $Mg_xZn_{1-x}O$ film growth at $x < 20\%$ on the Al_2O_3 substrates was $0.1 \dots 0.15 \text{ } \mu\text{m}/\text{hour}$. The thickness of films was determined by means of the interferometer МИИ-4 and changed from $0.1 \text{ } \mu\text{m}$ to $10 \text{ } \mu\text{m}$.

As a substrate for growing monocrystalline zinc oxide layers, single crystals of leicosapphire were used. In the hexagonal Al_2O_3 single crystals there is a plane that is perpendicular to z -axis that is designated (0001), and in rhombohedral ones – (111) [21]. From the possible variety of sapphire orientations for epitaxial growing the ZnO thin films, advantage was given to orientations with the densely packed planes (0001), (1102), (1120), (1012), on which it is possible to grow the layers with high mobility of charge carriers [21, 22].

By means of the spectrophotometer ИКС-29М and the use of facility ИПО-22 at $T = 300 \text{ K}$, the spectra of external reflection of Al_2O_3 substrate were measured within the range $400 \dots 1200 \text{ cm}^{-1}$. A mathematical model with the additive and phenomenological contribution of oscillators to permittivity was presented. The spectra of infrared reflection for $Mg_xZn_{1-x}O/Al_2O_3$, which allows to perform the dispersion analysis of spectra with account of orientation inherent to optical axes in film and substrate.

3. Theory and discussion of results

Let us consider the structure of $Mg_xZn_{1-x}O/Al_2O_3$ that consists of absorptive film on the absorptive semi-infinite substrate. The area of “residual rays” of ternary alloy $MgZnO$ comprises the range from 400 up to 1000 cm^{-1} . In the monographs [10, 25], there was shown the possibility to model semiconductor or dielectric structure that consists of optically-anisotropic (isotropic) film on the optically-anisotropic (isotropic) substrate, when using the multioscillometric mathematical model for the orientations $E \perp C$ and $E \parallel C$. In addition, calculation of spectra of infrared reflection from the $Mg_xZn_{1-x}O/Al_2O_3$ surface was carried out after formulas that take into account interaction of infrared emission with the phonon and plasma subsystems of film and semi-infinite substrate of Al_2O_3 for the case $E \perp C$ and $E \parallel C$:

$$RT(\nu) = \frac{(q_1^2 + h_1^2) \exp(\gamma_2) + (q_2^2 + h_2^2) \exp(-\gamma_2) + A \cos \delta_2 + B \sin \delta_2}{\exp(\gamma_2) + (q_1^2 + h_1^2) + (q_2^2 + h_2^2) \exp(-\gamma_2) + C \cos \delta_2 + D \sin \delta_2},$$

where

$$\begin{aligned} A &= 2(q_1 q_2 + h_1 h_2), \quad B = 2(q_1 h_2 + q_2 h_1), \\ C &= 2(q_1 q_2 + h_1 h_2), \quad D = 2(q_1 h_2 + q_2 h_1), \\ q_1 &= \frac{n_1^2 - n_2^2 - k_2^2}{(n_1 + n_2)^2 + k_2^2}, \quad q_2 = \frac{n_2^2 - n_3^2 + k_2^2 - k_3^2}{(n_2 + n_3)^2 + (k_2 + k_3)^2}, \\ h_1 &= \frac{2n_1 k_2}{(n_1 + n_2)^2 + k_2^2}, \quad h_2 = \frac{2(n_2 k_3 - n_3 k_2)}{(n_2 + n_3)^2 + (k_2 + k_3)^2}, \\ \gamma_2 &= \frac{4\pi k_2 d}{\lambda}, \quad \delta_2 = \frac{4\pi n_2 d}{\lambda} \end{aligned}$$

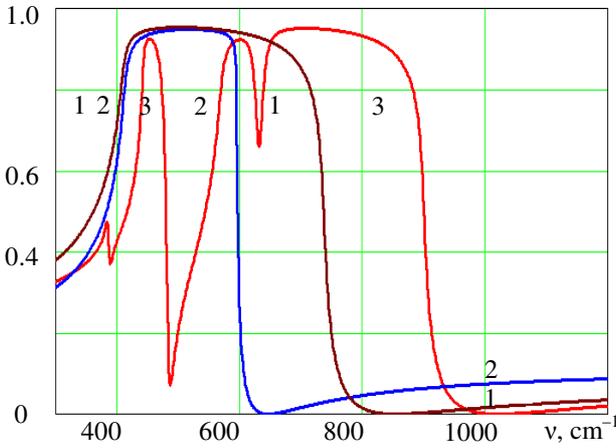
(n_1, n_2, n_3 are the indexes of refraction; k_1, k_2, k_3 – indexes of absorption inherent to air, film with the thickness d and semi-infinite substrate, respectively).

Table 1. Parameters of Al₂O₃ single crystal for calculation of $R(\nu)$ at the orientation $E \perp C$.

$\nu_{TOi}, \text{cm}^{-1}$	384	442	571	634
$\Delta\epsilon_i$	0.2	2.8	3.1	0.2
γ_{fi}/ν_{TOi}	0.015	0.01	0.2	0.02

Table 2. The mutually agreed volume parameters of single crystals of magnesium oxide [12, 26] and zinc oxide [10] ($T = 293 \text{ K}$).

ZnO	ϵ_0	ϵ_∞	ν_{TO}, cm^{-1}	ν_{LO}, cm^{-1}
ZnO ($E \perp C$)	8.1	3.95	412	591
ZnO ($E \parallel C$)	9.0	4.05	380	570
MgO ($E \perp C$)	2.98	9.39	416	738

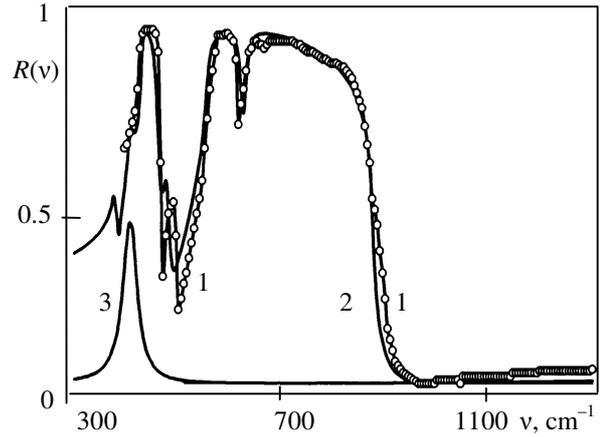

Fig. 1. Calculated spectra of infrared reflection $R(\nu)$ of single crystals MgO (1), ZnO (2), Al₂O₃ (3) at the orientation $E \perp C$.

Calculation of n_2 and n_3 was performed as based on the model of permittivity with additive contribution of active optical phonons ν_{TO} and plasmons ν_p [10, 25]:

$$\begin{aligned} \epsilon_{\text{MgZnO}}(\nu) &= \epsilon_{i1}(\nu) + j\epsilon_{2i}(\nu) = \\ &= \epsilon_{\infty i} + \frac{\epsilon_{\infty i}(\nu_{LOi}^2 - \nu_{TOi}^2)}{\nu_{TOi}^2 - \nu^2 - j\nu\gamma_{fi}} - \frac{\epsilon_{\infty i}\nu_{pi}^2}{\nu(\nu + j\gamma_{pi})} \end{aligned}$$

where ν_{LO}, ν_{TO} are the frequencies of longitudinal and transversal optical phonons; γ_f is the fading coefficient of optical phonon; γ_p and ν_p are fading coefficient and frequency of plasmon resonance; and $i = 1 \dots 3$ are indexes of oscillators in the film. When modeling the Al₂O₃ substrate, we used the dependence of permittivity of sapphire on frequency for $E \perp C$ [10]:

$$\epsilon(\nu) = \epsilon_\infty + \sum_{i=1}^4 \frac{\Delta\epsilon_i \nu_{TOi}^2}{\nu_{TOi}^2 - \nu^2 + j\nu\gamma_{fi}}, \quad (2)$$


Fig. 2. Spectra of infrared reflection $R(\nu)$ of zinc oxide film on substrate of Al₂O₃ single crystal of the orientation $E \perp C$: 1 – experiment ($d = 0.1 \mu\text{m}$); 2 – calculation of $R(\nu)$ at $\gamma_{f\perp} = 12 \text{ cm}^{-1}$, $\nu_{p\perp} = 480 \text{ cm}^{-1}$, $\gamma_{p\perp} = 800 \text{ cm}^{-1}$; 3 – calculation of $R(\nu)$ for ZnO film (without substrate).

where ϵ_∞ is a high-frequency permittivity of sapphire for the orientation $E \perp C$ (it was accepted to be equal to 3.2); $\Delta\epsilon_i$ is the force of i -th oscillator; ν_{TOi} – frequency of transversal optical fading of i -th oscillator; γ_{fi} is the value of fading coefficient of i -th oscillator. The data used for the calculation of spectra $R(\nu)$ from the Al₂O₃ surface were listed in Table 1.

In Fig. 1, the spectra of infrared reflection of single crystals of magnesium oxide (curve 1), zinc oxide (curve 2) and aluminium oxide (curve 3) at the orientation of $E \perp C$ are presented, which were measured with account of the data [10, 12]. For modeling the spectra of infrared reflection, the mathematical expressions of multioscillometric mathematical model (1) and (2) were used. The mutually agreed parameters of oscillators for the indicated single crystals are presented accordingly in Tables 1 and 2.

The area of “residual rays” of MgO, ZnO single crystals is located within the range 400 to 1000 cm^{-1} , which complicates task of exact determination of influence of optical parameters on characteristics of the reflection spectrum for every separately taken material. In addition, zinc oxide is a semiconductor where optical and electrophysical properties influence on the spectrum of reflection depending on the degree of doping the single crystal and type of charge carriers. It should be noted that each single crystal of presented in Fig. 1 ones was thoroughly studied by the authors earlier [10, 12].

To study the influence of properties inherent to optically-isotropic film on the spectrum of infrared reflection, the double-layer ZnO/Al₂O₃ and MgO/Al₂O₃ structures were used.

In Fig. 2, we show the experimental (points 1) and theoretical (curve 2) results of research of monocrystalline films of zinc oxide with the thickness 0.1 μm at $E \perp C$ by the methods of spectroscopy of infrared reflection. Experimental spectra were measured using the spectrometer ИКС-29М with the facility ИПО-22 (taking into account the method described in [10])

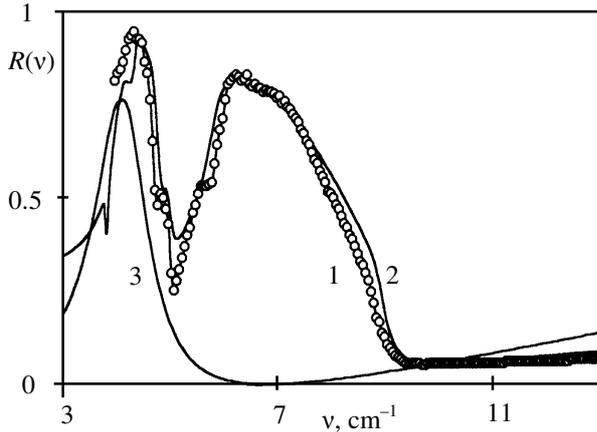


Fig. 3. Spectra $R(v)$ of the ZnO/Al₂O₃ structure: 1 – experiment ($d = 0.5 \mu\text{m}$); 2 – calculation of $R(v)$ at $\nu_{TO\perp} = 412 \text{ cm}^{-1}$, $\gamma_{f\perp} = 15 \text{ cm}^{-1}$, $\nu_{p\perp} = 400 \text{ cm}^{-1}$, $\gamma_{p\perp} = 870 \text{ cm}^{-1}$; 3 – calculation of $R(v)$ for ZnO film (without substrate).

within the range 400 to 1400 cm^{-1} . The spectra were registered in the polarized irradiation at the orientation of electric vector of $E \perp C$ of Al₂O₃ crystal. The curve 1 (points) corresponds to the experimental values of $R(v)$ of ZnO/Al₂O₃ structure with the thickness of ZnO layer $d = 0.1 \mu\text{m}$. The calculated spectrum from the ZnO/Al₂O₃ surface was measured at parameters for ZnO film, which were presented in signatures to Fig. 2 and data of Tables 1 and 2. As it is evident from the figure, in the spectrum there are minima at the frequencies 475, 505, 620 cm^{-1} . In the absence of ZnO film, minima in the Al₂O₃ spectra are at the frequencies 390, 420, 489, 633 cm^{-1} (Fig. 1, curve 3).

It is shown in theory that when the thickness is less than 80 nm, the shape of the spectrum $R(v)$ is defined mainly by Al₂O₃ substrate, and the zinc oxide layer of the thickness 10 μm forms the spectrum of reflection of semi-infinite zinc oxide single crystal. The change in sample orientation in the polarized radiation did not change practically the shape of spectrum $R(v)$, which testified that the orientation of the textured ZnO layers is the same as in the substrate. The curve 3 of Fig. 2 was calculated for free film of zinc oxide with the thickness $d = 0.1 \mu\text{m}$. The peak of the curve is at the frequency 412 cm^{-1} at $R(v) = 0.47$.

In Fig. 3, the spectra of infrared reflection of ZnO/Al₂O₃ structure at the orientation $E \perp C$ are presented. The curve 1 corresponds to $R(v)$ when the thickness of ZnO layer $d = 0.5 \mu\text{m}$. In the spectrum, there is a minimum of reflection at the frequency 510 cm^{-1} (curve 1) and two bends near 430 and 600 cm^{-1} , while when modeling the ZnO/Al₂O₃ structure, minima of $R(v)$ are at the frequencies 325, 427, 491 and 515 cm^{-1} (curve 2).

The maxima of $R(v)$ are located at the frequencies 432 and 600 cm^{-1} , here a curve fluently diminishes $R(v)$ into the area of higher frequencies. The calculated $R(v)$ (curve 2) is determined for the following parameters of ZnO layer: $d = 0.5 \mu\text{m}$, $\nu_{TO\perp} = 412 \text{ cm}^{-1}$, $\gamma_{f\perp} = 15 \text{ cm}^{-1}$,

$\nu_{p\perp} = 400 \text{ cm}^{-1}$, $\gamma_{p\perp} = 870 \text{ cm}^{-1}$. On the curve 3, the theoretical spectrum of $R(v)$ of free ZnO film is shown at the parameters above indicated. The maximum $R(v) = 0.76$ is at the frequency 415 cm^{-1} .

As seen from Fig. 3, the presence in ZnO films of free charge carriers (electrons) of the order of $n_0 = 10^{18} \dots 10^{19} \text{ cm}^{-3}$ substantially deforms the spectrum of reflection in the area between 400 and 1000 cm^{-1} . The reflection coefficient at the frequency 680 cm^{-1} diminishes to 0.8 at the presence of the minimum 0.4 at the frequency 510 cm^{-1} .

The change of position of the doped zinc oxide films on Al₂O₃ substrate in the plane xy practically does not change the shape of $R(v)$ spectrum, which testifies isotropy of optical and electrophysical properties of the investigated system. In addition, it is possible to assert that the optical axis of the textured layers of zinc oxide and sapphire is normal to the plane of xy ($C \perp xy$).

For the concentration of free charge carriers $n_0 > 5 \cdot 10^{17} \text{ cm}^{-3}$, there is decreasing the reflection coefficient at the frequencies higher than 700 cm^{-1} . On the basis of analysis of the studied ZnO/Al₂O₃ structures, it is found that in our case the zinc oxide layers have the following values of the electron concentration $n_0 = (1.6 \dots 2.8) \cdot 10^{18} \text{ cm}^{-3}$, mobility $\mu = 1.1 \dots 3.1 \text{ cm}^2/(\text{V}\cdot\text{s})$ and conductivity within the range $\sigma_0 = 110 \dots 200 \text{ Ohm}^{-1}\cdot\text{cm}^{-1}$.

In Fig. 4, the calculated dependences $R(v)$ of MgO/Al₂O₃ structure on the thickness of magnesium oxide film are presented. The curves 2 to 4 correspond to the thickness 0.1, 0.25, 0.5 μm at $\gamma_{f\perp} = 12 \text{ cm}^{-1}$. The increase of the film thickness to 0.5 μm results in the considerable increase of $R(v)$ values in the area close to 500 cm^{-1} . Within the frequency range from 450 to 580 cm^{-1} , there is a change of $R(v)$ from 0.18 for $d = 0.1 \mu\text{m}$ (curve 2) to 0.45 for $d = 0.5 \mu\text{m}$ (curve 4). The curve 1 was calculated for the Al₂O₃ single crystal for parameters indicated in Table 1. The change of film thickness from 0.1 to 0.5 μm at the unchanged mutually agreed parameters for magnesium oxide is not accompanied by changes in the spectrum of reflection within the range 600...1200 cm^{-1} .

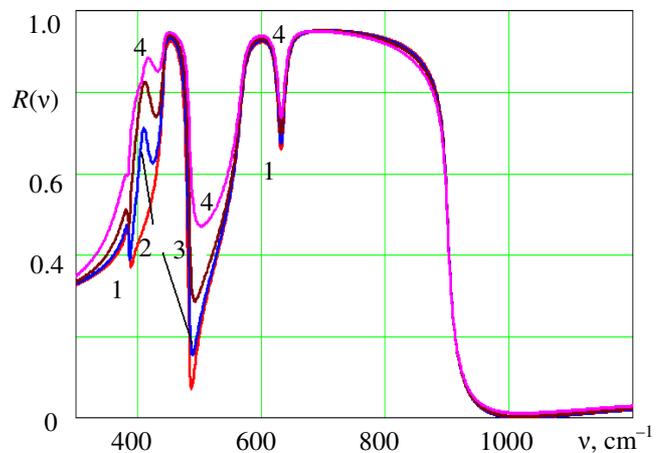


Fig. 4. Calculation spectra $R(v)$ of the MgO/Al₂O₃ structure: 2–4 – calculation of $R(v)$ at $\nu_{TO\perp} = 416 \text{ cm}^{-1}$ and $\gamma_{f\perp} = 12 \text{ cm}^{-1}$, $d = 0.1 - 0.5 \mu\text{m}$; 1 – calculation of $R(v)$ for Al₂O₃ (without film).

Table 3. Parameters of the investigated samples.

Sample	ϵ_{∞}	ϵ_0	$\nu_{TO1}, \text{cm}^{-1}$	$\nu_{LO1}, \text{cm}^{-1}$	ΔS_1	$\gamma_{f1}, \text{cm}^{-1}$	$\nu_{TO2}, \text{cm}^{-1}$	$\nu_{LO2}, \text{cm}^{-1}$	ΔS_2	$\gamma_{f2}, \text{cm}^{-1}$	$\nu_{TO3}, \text{cm}^{-1}$	$\gamma_{f3}, \text{cm}^{-1}$
$\text{Mg}_{0.47}\text{Zn}_{0.53}\text{O}/\text{Al}_2\text{O}_3$	3.3	7.06	385	386	1.5	5.0	436	636	15	20	730	40
$\text{Mg}_{0.47}\text{Zn}_{0.53}\text{O}/\text{Al}_2\text{O}_3$	3.1	7.88	389	395	0.8	9.0	447	702	7.0	10	728	20

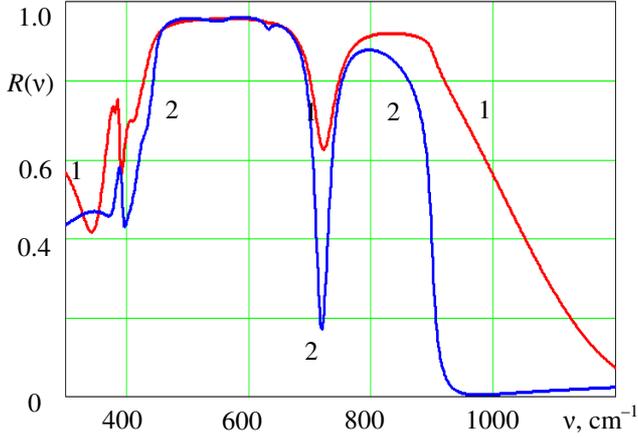


Fig. 5. Calculated spectra $R(\nu)$ of the $\text{Mg}_x\text{Zn}_{1-x}\text{O}/\text{Al}_2\text{O}_3$ structure: 1 – $x = 0.47$; 2 – $x = 0.60$ at $d = 2 \mu\text{m}$.

Fig. 5 shows the dependence of $R(\nu)$ of the $\text{Mg}_x\text{Zn}_{1-x}\text{O}/\text{Al}_2\text{O}_3$ structure at $x = 0.47$ (curve 1) and $x = 0.60$ (curve 2) with the film thickness $2 \mu\text{m}$. This calculation was performed using the Kramers–Kronig relations and data [25] and presented in Table 3. The values of static dielectric constant listed in Table 3 were determined by the authors of this paper with the use of the Liden–Sax–Teller relation. The obtained results are well agreed with the data presented in the plot of the work [25]. As it is obvious from comparison of the curves 1 and 2, the increase of Mg content in the $\text{Mg}_x\text{Zn}_{1-x}\text{O}/\text{Al}_2\text{O}_3$ structure from $x = 0.47$ (curve 1) up to 0.60 (curve 2) is accompanied by changes in the spectrum of external reflection at the frequencies of “residual rays” of zinc oxide and magnesium oxide.

The most essential changes are observed accordingly in the ranges $650\dots750$ and $900\dots1100 \text{cm}^{-1}$, which is caused by the frequencies of transversal and longitudinal optical phonons in the investigated materials. In turn, it indicates the possibility to develop practical modulators for the infrared spectral range.

Fig. 6 shows the dependence of $R(\nu)$ of the $\text{Mg}_x\text{Zn}_{1-x}\text{O}/\text{Al}_2\text{O}_3$ structure on the thickness of $\text{Mg}_x\text{Zn}_{1-x}\text{O}$ film. The curves 1 to 3 correspond to the thickness $1, 0.5, 0.25 \mu\text{m}$. The calculation was performed with the parameters presented in Table 3. As seen from the figure, the increase of film thickness from 0.25 to $1 \mu\text{m}$ results in the considerable increase of $R(\nu)$ in the whole range of “residual rays”. At the frequency 525cm^{-1} , there is a change of $R(\nu)$ from 0.59 for $d = 0.25$ to 0.92 for $d = 1 \mu\text{m}$, for the frequency 726cm^{-1} the increase of $R(\nu)$ is observed from 0.63 for $d = 0.25 \mu\text{m}$ to

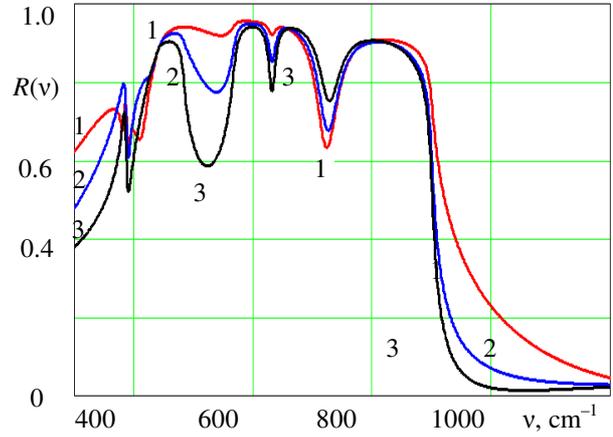


Fig. 6. Theoretical spectra of reflection $R(\nu)$ of the $\text{Mg}_x\text{Zn}_{1-x}\text{O}/\text{Al}_2\text{O}_3$ structure at $x = 0.47$: $d = 1, 0.5, 0.25 \mu\text{m}$ (1–3).

0.77 for $d = 1 \mu\text{m}$. Most essential changes from 0.08 to 0.4 were registered at the frequency 940cm^{-1} .

4. Conclusions

Thus, obtained in this work by using the method of infrared spectroscopy of external reflection are optical characteristics of thin films of ternary alloys $\text{Mg}_x\text{Zn}_{1-x}\text{O}$ on the Al_2O_3 dielectric substrate in the area of “residual rays” of film and substrate. It has been shown that the changes in film thickness and content of Mg substantially deform the spectrum of reflection in the area of “residual rays” of film and substrate, decrease reflection ability. The computer experiment of infrared spectra allowed to determine the static dielectric constant of $\text{Mg}_x\text{Zn}_{1-x}\text{O}$ structure at the different x values for the orientation $E \perp C$. It is found that the $\text{Mg}_x\text{Zn}_{1-x}\text{O}/\text{Al}_2\text{O}_3$ structures is well modeled with using the mutually agreed parameters presented in Tables 1 to 3, for the single crystals of magnesium oxide, zinc oxide and leucosapphire for the orientation $E \perp C$, which confirms perspectives of the non-destructive method of infrared spectroscopy for determination of optical characteristics of films of ternary alloys and rate of their texturing.

Acknowledgement

The work was carried out within the framework of theme No 89452 “Influence of doping on structural, optical and electron-phonon properties and stability of anisotropic crystals” with financial support of the Ministry of Education and Science of Ukraine.

References

- Özgür Ü., Alivov Ya.I., Liu C., Teke A., Reshchikov M.A., Doğan S., Avrutin V., Cho S.-J. and Morkoç H. A comprehensive review of ZnO materials and devices. *J. Appl. Phys.* 2005. **89**. P. 041301.
- Djurišić A.B., Ng A.M.C. and Chen X.Y. ZnO nanostructures for optoelectronics: Material properties and device applications. *Prog. Quant. Electron.* 2010. **34**. P. 191–259.
- Moezzi A., McDonagh A.M. and Cortie M.B. Zinc oxide particles: Synthesis, properties and applications. *Chem. Eng. J.* 2012. **185-186**. P. 1–22.
- Ievtushenko A.I., Lashkarev G.V., Lazorenko V.I., Karpyna V.A. and Khranovskyy V.D. ZnO-based detectors of ultraviolet radiation (Review). *Phys. Chem. Solid State.* 2008. **9**. P. 869–882.
- Scheer R. and Schock H.-W. *Chalcogenide Photovoltaics: Physics, Technologies, and Thin Film Devices*. WILEY-VCH Verlag GmbH & Co. KGaA, 2011.
- Abou-Ras D., Kirchartz T. and Rau U. *Advanced Characterization Techniques for Thin Film Solar Cells*. WILEY-VCH Verlag GmbH & Co. KGaA, 2011.
- Kovtun N.A., Boyko B.T., Khyapunov G.S. and Kopach V.R. Electrical properties of transparent polycrystalline ZnO:Al films prepared by magnetron sputtering. *Problems of atomic science and technology*. 1999. **10**, No 2. P. 75–78.
- Mykhalichko B.M. *General Chemistry: Theoretical Bases*. Kyiv, Znannya, 2009 (in Ukrainian).
- Ostroushko A.A. *Physico-Chemical Fundamentals of Solid-State Materials for Electronics and Catalysis*: Tutorial. Ural University Publ., 2011 (in Russian).
- Venger E.F., Melnichuk O.V., Pasechnik Yu.A. *Spectroscopy of Residual Rays*. Naukova dumka, Kyiv, 2001 (in Russian).
- Jin Ch. *Growth and Characterization of ZnO and ZnO-Based Alloys: Mg_xZn_{1-x}O and Mn_xZn_{1-x}O*, Ph.D Thesis. North Carolina State University, Raleigh, 2003.
- Venger E.F., Yevtushenko A.I., Korbutyak D.V., Melnichuk L.Yu and Melnichuk O.V. Investigation of magnesium oxide using IR spectroscopy. Physical and mathematical notes: *Collection of research works*. Nizhyn: Publ. House of Mykola Gogol State University of Nizhyn, 2010. P. 53–58.
- Ohtomo A., Kawasaki M., Koida T., Masubuchi K., Koinuma H., Sakurai Y., Yoshida Y., Yasuda T. and Segawa Y. Mg_xZn_{1-x}O as a II–VI widegap semiconductor alloy. *Appl. Phys. Lett.* 1998. **72**. P. 2466–2468.
- Makino T., Segawa Y., Kawasaki M., Ohtomo A., Tamura K., Yasuba T. and Koinuma H. Band gap engineering based on Mg_yZn_{1-x}O and Cd_yZn_{1-y}O ternary alloy films. *Appl. Phys. Lett.* 2001. **78**. P. 1237–1239.
- Janotti A., Van de Walle C.G. Fundamentals of zinc oxide as a semiconductor. *Rep. Prog. Phys.* 2009. **72**. 126501 (29 p.).
- Schleife A., Rödl C., Furthmüller J. and Bechstedt F. Electronic and optical properties of Mg_xZn_{1-x}O and Cd_xZn_{1-x}O from *ab initio* calculations. *New Journal of Physics*. 2011. **13**. 085012 (<http://www.njp.org/>).
- Ohtomo A., Tamura K., Kawasaki M., Makino T., Segawa Y., Tang Z.K., Wong L.G.K., Matsumoto Y. and Koinuma H. Room-temperature stimulated emission of excitons in ZnO/(Mg, Zn)O superlattices. *Appl. Phys. Lett.* 2000. **77**. P. 2204–2206.
- Jin Y., Zhang B., Shuming Y., Wang Y., Chen J., Zhang H., Huang C., Cao C., Cao H. and Chang R.P.H. Room temperature UV emission of Mg_xZn_{1-x}O films. *Solid State Commun.* 2001. **119**. P. 409–413.
- Makino T., Segawa Y., Ohtomo A., Tamura K. and Koinuma H. Band gap engineering based on Mg_xZn_{1-x}O ternary alloy films. *Appl. Phys. Lett.* 2001. **78**. P. 1237–1239.
- Gruber Th., Kirchner C., Kling R., Reuss F. and Waag A. ZnMgO epilayers and ZnO–ZnMgO quantum wells for optoelectronic applications in the blue and UV spectral region. *Appl. Phys. Lett.* 2004. **84**. P. 5359–5361.
- Ruby and Sapphire*. M.V. Klassen-Neklyudova, Kh.S. Bogdasarov (Eds.). Moscow, Nauka, 1974 (in Russian).
- Venger E.F., Melnichuk A.V., Pasechnik Ju.A., Sukhenko E.I. IR Spectroscopy studies of the zinc oxide on sapphire structure. *Ukr. J. Phys.* 1997. **42**, No 11. P. 1357–1360.
- Ukhanov Yu.I. *Optical Properties of Semiconductors*. Moscow, Nauka, 1977 (in Russian).
- Hofmeister M., Keppel E. and Speck A.K. Absorption and reflection infrared spectra of MgO and other diatomic compounds. *Monthly Notices of the Royal Astronomical Society*. 2003. **345**. P. 16–38.
- Chen J. and Shen W.Z. Long-wavelength optical phonon properties of ternary MgZnO thin films. *Appl. Phys. Lett.* 2003. **83**. P. 2154–2156.

Authors and CV



Venger Yevgen Fedorovich. Doctor of Physics and Mathematics Sciences, Professor, Corresponding Member of the National Academy of Sciences of Ukraine, Department of Physical and Technical Problems of Energetics. His scientific works are devoted to semiconductor electronics and optoelectronics. He is one of the founders of the polariton optoelectronics direction. Ye.F. Venger has more than 500 publications, 40 patents, 24 textbooks and manuals. The area of scientific interests includes physics and technology of semiconductor materials, hetero- and hybrid structures and devices (thin-film solar cells, photoresistors, new types of photoconverters, in particular, efficient, wide-band and selective short-wave radiation sensors, *etc.*), as well as analysis, diagnostics, modeling and forecasting the physical processes in different objects. *Head of the Department of Semiconductor Heterostructures at the V. Lashkaryov Institute of Semiconductor Physics, NAS of Ukraine.*
E-mail: vengeref@gmail.com



Venger Iryna Vsevolodivna

Researcher at the Department of Physical and Technological Foundations of Sensor Material Science at the V. Lashkaryov Institute of Semiconductor Physics of the National Academy of Sciences of Ukraine. The author of over 30 publications, 4 textbooks and manuals. The area of her scientific interests includes modeling the optical and electrophysical properties in polar optically-isotropic and anisotropic semiconductors and structures on their basis.

E-mail: vengeriv@nas.gov.ua



Korsunskaya Nadiya Ovsyivna.

Doctor of Physics and Mathematics, Professor, Laureate of the State Prize of the Ukrainian SSR.

Her scientific works are devoted to the study of recombination and electronically stimulated diffusion processes and defect drift processes in

semiconductors and dielectrics, as well as processes of degradation of materials and devices. The area of scientific interests covers physics and technology of semiconductor materials, including nanostructured materials. The author of more than 300 scientific works, 7 author's certificates and 2 patents in the field of semiconductor and dielectric physics.

Leading researcher at the V. Lashkaryov Institute of Semiconductor Physics, NAS of Ukraine.

E-mail: Korsunskaya@ukr.net



Melnichuk Liudmyla Yuriyivna

Candidate of Physical and Mathematical Sciences, Associate Professor, Excellence in Education of Ukraine.

In 1996 she defended her Ph.D. thesis "Anisotropy of surface plasmon-phonon polaritons in single crystals of zinc oxide" by the specialty "Solid State Physics". In April 1998, she was awarded the title of Associate Professor. She is the author of more than 120 scientific and methodological works in the area of physics of semiconductors and dielectrics, solid state physics, problems of higher education.

Head of the Department of Physics, at the Mykola Gogol Nizhyn State University.

E-mail: lyu.melnichuk@gmail.com



Melnichuk

Olexander

Volodymyrovych Doctor of Physical and Mathematical Sciences, Professor, Excellence in Education of Ukraine. In 2001 he defended his doctoral dissertation "Surface Plasmon-Phonon Excitements in Univalent Semiconductors ZnO and

6H-SiC and Structure Based on them" in the area of "Physics of Semiconductors and Dielectrics". In April 2002, he was awarded the title of professor. He is the author of over 300 scientific and methodological works in the area of physics of semiconductors and dielectrics, solid state physics, mathematical modeling, problems of higher and secondary schools.

Vice-Rector for Scientific and International Relations at the Mykola Gogol Nizhyn State University.

E-mail: mov310310@gmail.com



Khomenkova Larisa Yuriyivna

Candidate of Physics and Mathematics, Senior Researcher. The main area of activity is creation of multifunctional composite materials and study of their properties for applying in microelectronics and light emitting devices. She is the author of

more than 150 scientific publications in the area of solid state physics.

Senior Researcher at the V. Lashkaryov Institute of Semiconductor Physics, NAS of Ukraine.

E-mail: khomen@ukr.net